

Methyl formate  
107-31-3 | DTXSID5025609

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $3.44\text{e-}13$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:**  $4.28\text{e-}01$

**Confidence level:**  $6.93\text{e-}01$

## Nearest Neighbors from the Training Set

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Methyl formate

**Measured:**  $2.27\text{e-}13$

**Predicted:**  $3.44\text{e-}13$

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Ethyl formate

**Measured:**  $1.02\text{e-}12$

**Predicted:**  $1.05\text{e-}12$

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Formic acid, propyl ester

**Measured:**  $2.38\text{e-}12$

**Predicted:**  $1.78\text{e-}12$

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tert-Butyl formate

**Measured:**  $7.37\text{e-}13$

**Predicted:**  $1.01\text{e-}12$

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Formic acid, butyl ester

**Measured:**  $3.12\text{e-}12$

**Predicted:**  $2.12\text{e-}12$